# VALIDATING PHYSICS SIMULATION CODES

ASSESSING THE PREDICTIVE CAPABILITIES OF SIMULATIONS

The Continuum Dynamics Group develops numerical methods, algorithms, and physical models for simulating physical phenomena. Critical to building confidence in physics simulation codes is validation, the process of determining, by quantitative comparison, how well code predictions agree with the actual behavior of physical systems. The experimental data can range in complexity from a simple curve representing temperature versus time to images of intricate patterns in a shock-tube experiment. Analysis of complex behavior is challenging. To meet such challenges, we are developing advanced techniques that combine physics principles with applied mathematics and statistics.

Physics simulation codes are built from component models, each describing a distinct aspect of physical behavior. For example, one model might describe the cooling of a liquid metal and another, its solidification. Uncertainties in both the experimental results and the simulation, including calculational errors in the simulation, must be considered when inferring the model parameters, which are used to estimate uncertainties in simulation predictions.

Within a unifying validation framework, we strive to understand the models contained in the simulation code and lay the foundation for quantifying a code's predictive capability. The ultimate goal is to ensure that the simulation code and its models are consistent with the full hierarchy of experiments, ranging from basic experiments involving individual models up to more complex experiments involving combinations of models.

temperature

1573
1453
1333
1213
1093
973

thermocouple
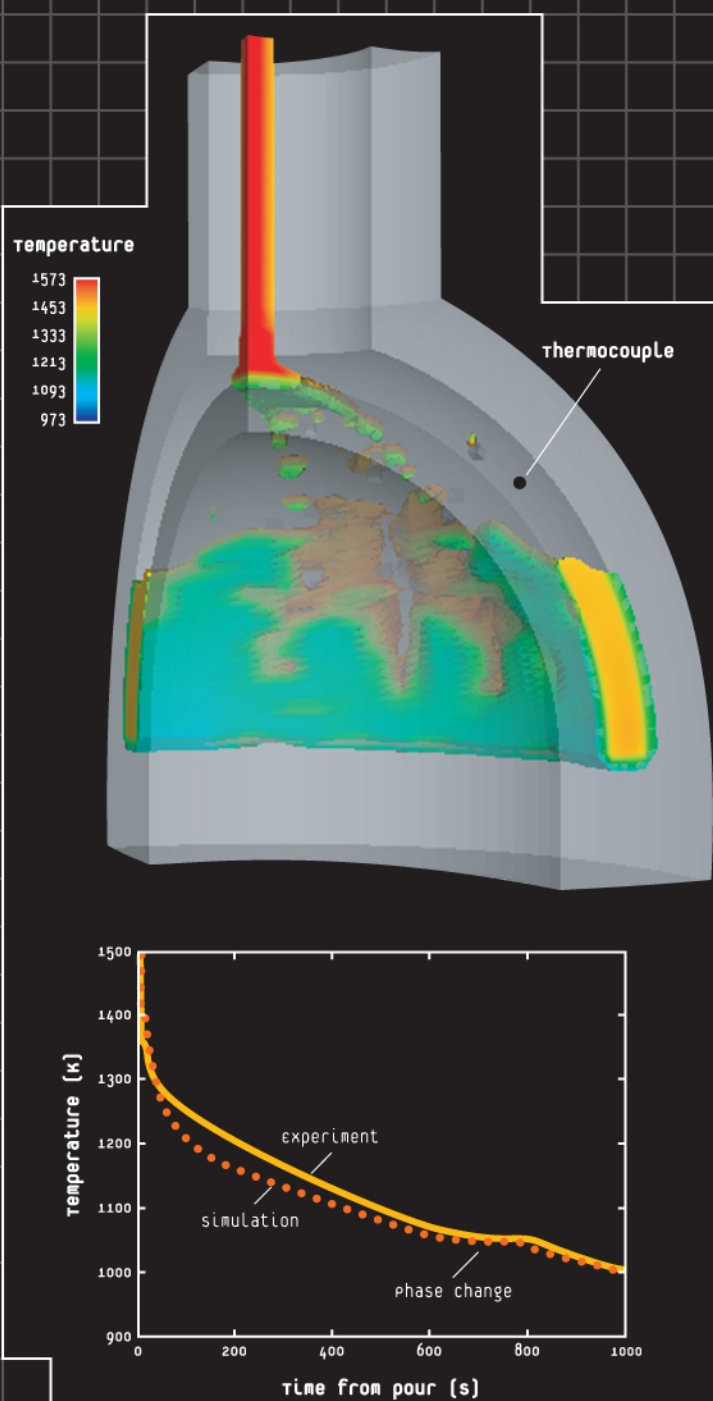
### simulating uranium casting with the Truchas code

Above is a simulation of the casting of a hemisphere of depleted uranium, performed with the Truchas code. The graph compares the predicted cooling curve with the experimental measurements. Both show a phase change at about 700 seconds.

estimating PTW fit uncertainties

(Left) The fit of the Preston-Tonks-Wallace (PTW) plastic-deformation model (solid lines) to experimental data (points) for tantalum is based on detailed estimates of experimental uncertainties. (Right) The degree of uncertainty in the stress-strain behavior, visualized as a set of Monte Carlo–generated curves for three experimental conditions is consistent with the data.
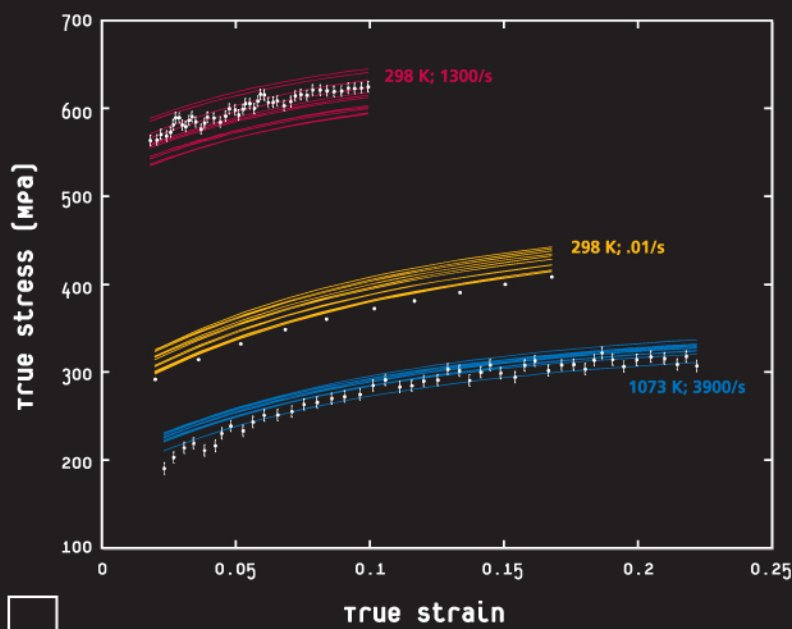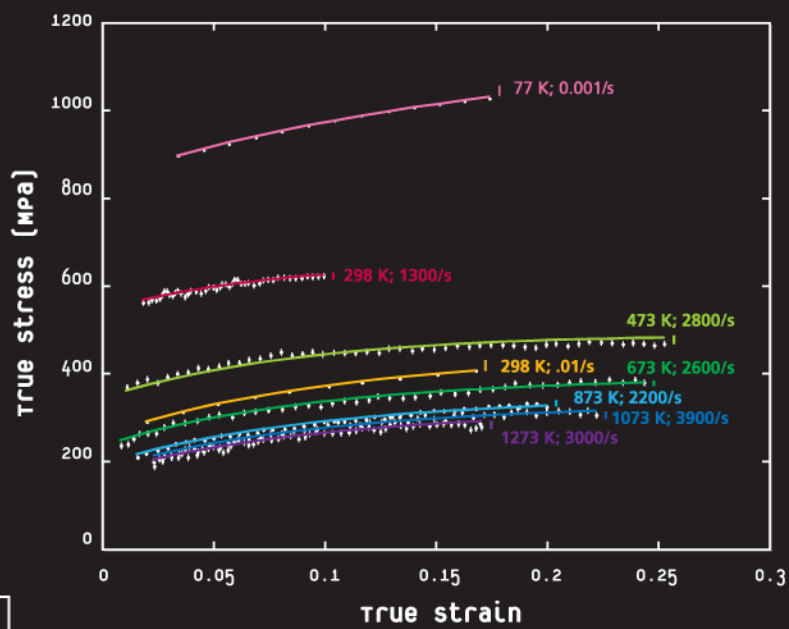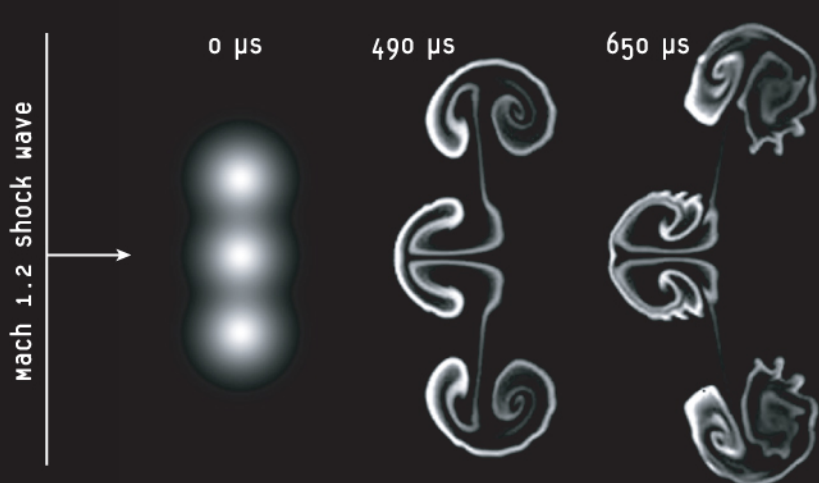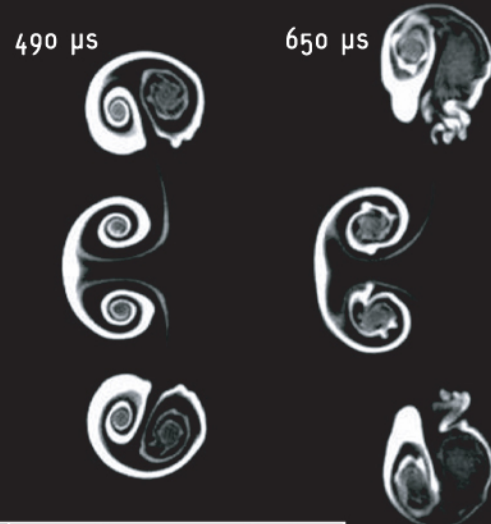
predicting shock-induced mixing with the cuervo code

Predictions (left) made with the Cuervo hydrodynamic code before a shock-tube experiment involving sulfur hexafluoride cylinders (three bright spots) were based on nominal experimental conditions. Experimental results (right), obtained with planar laser-induced fluorescence, illustrate Richtmyer-Meshkov fluid instabilities. The Cuervo predictions agree qualitatively with the experimental images, yet they differ in detail.

Kenneth M. Hanson, CCS-2
kmh@lanl.gov, 505-667-1402

The World's Greatest Science
Protecting America

NNSA

Los Alamos
NATIONAL LABORATORY
ESTABLISHED 1943